Benzamide, 2-bromo-N-ethyl-N-butyl-

Inchi: InChI=1S/C13H18BrNO/c1-3-5-10-15(4-2)13(16)11-8-6-7-9-12(11)14/h6-9H,3-5,10H2,1-
InchiKey: KNFQWDAKTKPAJP-UHFFFAOYSA-N
Formula: C13H18BrNO
SMILES: CCCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 284.19

Physical Properties

Property code	Value	Unit	Source
gf	157.54	kJ/mol	Joback Method
hf	-105.31	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.711		Crippen Method
mcvol	199.320	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	660.97	K	Joback Method
tc	875.74	K	Joback Method
tf	417.41	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.84	J/mol×K	660.97	Joback Method
cpg	511.75	J/mol×K	696.77	Joback Method
cpg	525.69	J/mol×K	732.56	Joback Method
cpg	538.70	J/mol×K	768.36	Joback Method
cpg	550.85	J/mol×K	804.15	Joback Method
cpg	562.20	J/mol×K	839.95	Joback Method
cpg	572.79	J/mol×K	875.74	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume